Curriculum Vitae

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Personal Information

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Education

Ph.D.: Biochemistry, Rutgers University, New Brunswick, NJ
Advisor: Professor Regina Pietruszko
Degree conferred: August, 1985

B.S.: Chemistry, University of Hawaii, Honolulu, HI
Degree conferred: May, 1981

A.S.: Biology, Gloucester County College, Sewell, NJ
Degree conferred: May, 1979

Employment Experience

3/08 to Present	**Grollman-Glick Professor of Pharmaceutical Sciences**, University of Maryland, Baltimore, School of Pharmacy, Department of Pharmaceutical Sciences, 20 Penn Street, Baltimore, MD 21201, USA
4/12 to Present	**Co-Founder and Chief Scientific Officer**, SilcsBio, LLC, BioPark 801 West Baltimore Street Suite 516, Baltimore, MD 21201, USA
4/12 to Present	**Adjunct Professor**, University of Maryland, Baltimore, School of Medicine, Department of Anesthesiology, Baltimore, MD 21201, USA
5/04 to 3/08	**Professor**, University of Maryland, Baltimore, School of Pharmacy, Department of Pharmaceutical Sciences, 20 Penn Street, Baltimore, MD 21201, USA
8/02 to Present	**Director**, Computer-Aided Drug Design Center, University of Maryland, School of Pharmacy, 20 Penn Street, Baltimore, MD 21201, USA
6/97 to 5/04	**Associate Professor**, University of Maryland, Baltimore, School of Pharmacy, Department of Pharmaceutical Sciences
1/02 to 6/02	**Visiting Professor**, The Scripps Research Institute, Department of Molecular Biology, TPC6, 10550 North Torrey Pines Road, LaJolla, CA 92037, USA
9/95 to Present	**Member of the Program in Experimental Therapeutics**, Greenebaum Cancer Center, University of Maryland, Baltimore, MD 21201, USA
6/93 to 6/97	**Assistant Professor:** University of Maryland at Baltimore, School of Pharmacy, Department of Pharmaceutical Sciences, 20 North Pine Street, Baltimore, MD 21201, USA
9/92 to 6/93	**Visiting Assistant Professor:** Swarthmore College, Department of Chemistry, 500 College Ave., Swathmore, PA 19081, USA
4/88 to 7/92	**Research Associate:** Harvard University, Department of Chemistry, 12 Oxford Street, Cambridge, MA 02138, USA Supervisor: Prof. Martin Karplus
9/90 to 6/93	**Consultant:** Polygen Corporation, 200 Fifth Avenue, Waltham, MA 02254, USA
1/86 to 3/88	**Postdoctoral Fellow:** Karolinska Institutet, Department of Medical Biophysics, S104-01, Stockholm, Sweden. Supervisor: Prof. Rudolf Rigler
9/81 to 12/85	**Biochemistry Research Assistant:** Rutgers University, Biochemistry

Graduate Program, New Brunswick, NJ, USA,
Supervisor: Prof. Regina Pietruszko

11/79 to 6/81 **Lab Assistant:** University of Hawaii, Hawaii Institute of Geophysics, Honolulu, HI, USA. Supervisor: Prof. Donald Thomas

Advisory Boards/Steering Committees

Lawrence Livermore National Laboratory Biosciences Directorate
Unihart Biotech Pharma N.V.
National Resource for Biomedical SuperComputing, Pittsburgh, PA
Accelrys Inc.
Environmental Sciences Division, Oak Ridge National Laboratory
Science Gateway Institute, NSF's S2I2 program

Scientific, Professional and Scholarly Organizations

Federation of American Societies for Experimental Biologies (1988-present)
American Society for Biochemistry and Molecular Biology (1988-1999)
Biophysical Society (2000-present)
American Chemical Society (1992-present)
American Association of Colleges of Pharmacy (1992-1998)
International Society of Quantum Biology and Pharmacology (1992-present)
- Vice President: 2004
- President: 2005-2006
- Web host: 2005-present

American Association for the Advancement of Science (1995-present)
Rho Chi Honor Society (1993-present)

Editorial Board Member

Proteins: Structure, Function, and Bioinformatics
Journal of Computational Chemistry
PLoS Computational Biology
Advances and Applications in Bioinformatics and Chemistry
Open Access Bioinformatics
Drug Design Reviews, 2002 to 2005

Journals Reviewed For

Biophysical Journal
Bioorganic & Medicinal Chemistry Letters
Biochemistry
Biopolymers
Carbohydrate Research
ChemiPhys Chemi

Journal of Computational Physics
Journal of the American Chemical Society
Journal of Biomolecular Structure and Dynamics
Journal of Computational Chemistry
Journal of Computer-Aided Molecular Modeling
Journal of Chemical Information and Modeling
Journal of Chemical Physics
Journal of Chemical Theory and Computation
Journal of Medicinal Chemistry
Journal of Molecular Graphics and Modeling
Journal of Physical Chemistry
Langmuir
Nucleic Acids Research
Physical Chemistry Chemical Physical
Peptides
Proteins
Proceedings of the Indian National Science Academy
RNA

Honors and Awards

NSF NATO Postdoctoral Research Fellowship, 1987
Karolinska Fellowship for Foreign Researchers, 1986-1987
NIH Postdoctoral Fellowship, 1988-1990
Alumnus of the Years, Gloucester County College, Sewell, NJ, ca. 1992
NSF European Centre for Atomic and Molecular Computations Fellowship, 1997
Maryland Chemist of the Year 2006: MD Chapter of the American Chemical Society
Researcher of the Year, University of Maryland, Baltimore, 2012
Inaugural Member, Gloucester County College Hall of Fame, Sewell, NJ, 2013

Publications in Refereed Journals

1. MacKerell, A.D., Jr., Vallari, R.C. and Pietruszko, R., Human mitochondrial aldehyde dehydrogenase inhibition by diethyldithiocarbamic acid methanethiol mixed disulphide: A derivative of disulfiram., **FEBS Letters** 179:77-81, 1985
2. MacKerell, A.D., Jr., Blatter, E.E. and Pietruszko, R., Human aldehyde dehydrogenase: Kinetic identification of the isozymes for which biogenic aldehydes and acetaldehyde compete. **Alcoholism: Clinical and Experimental Research** 10:266-277, 1986
3. MacKerell, A.D., Jr., McWright, R.S. and Pietruszko, R., Bromoacetophenone as an affinity reagent for human aldehyde dehydrogenase. **Biochemistry** 25:5182-5189, 1986
4. MacKerell, A.D., Jr., and Pietruszko, R., Chemical modification of human aldehyde dehydrogenase by substrate., **Biophysica Biochemica Acta** 911:306-317, 1986

5. MacKerell, A.D., Jr., Rigler, R., Nilsson, L., Hahn, U. and Saenger, W., Protein Dynamics: A time-resolved fluorescence, energetic and molecular dynamics study of ribonuclease T1. **Biophysical Chemistry** 26:247-261, 1987
6. Abriola, D.P., Fields, R., Stein,S., MacKerell, A.D., Jr. and Pietruszko, R., Active-site identification of human aldehyde dehydrogenase., **Biochemistry**, 26:5679-5684, 1987
7. MacKerell, A.D., Jr., Nilsson, L., Rigler, R. and Saenger, W., Molecular dynamic simulations of ribonuclease T1: Analysis of the effect of solvent on the structure, fluctuations and active site of the free enzyme., **Biochemistry,** 27:4547-4556, 1988
8. MacKerell, A.D., Jr., Molecular modeling and dynamics of neuropeptide Y. **Journal of Computer-Aided Molecular Design** 2:55-63, 1988
9. MacKerell, A.D., Jr., Rigler, R., Nilsson, L., Heinemann, U. and Saenger, W., Molecular dynamic simulations of ribonuclease T1: Effect of solvent on the interaction with 2'GMP., **European Biophysics Journal** 16:287-297, 1988
10. MacKerell, A.D., Jr., Hemsen, A., Lacroix, J.S. and Lundberg, J.M., Analysis of structure-function relationships of neuropeptide Y using molecular dynamics simulations and pharmacological activity measurements., **Regulatory Peptides** 25:295-313, 1989
11. MacKerell, A.D., Jr., Nilsson, L., Rigler, R. Heinemann, U. and Saenger, W., Molecular dynamic simulations of ribonuclease T1: Comparison of the free enzyme and the 2'GMP-enzyme complex., **Proteins: Structure, Function and Genetics** 6:20-31, 1989
12. Chen, E., Soderberg, P.G., MacKerell, A.D., Jr., Lindstrom, B. and Tengroth, B.M., Inactivation of lactate dehydrogenase by UV radiation in the 300 nm wavelength region., **Radiation and Environmental Biophysics** 28:185-191. 1989.
13. Abriola, D.P., MacKerell, A.D., Jr. and Pietruszko, R., Human aldehyde dehydrogenase: Correlation of activity loss with ^{14}C-bromoacetophenone into glutamate 268 and cysteine 302; Quarter-of-the-sites reactivity of aldehyde dehydrogenase., **Biochemical Journal** 266:179-187, 1990.
14. MacKerell, A.D., Jr., Rigler, R., Hahn, U. and Saenger, W., Thermodynamic analysis of the equilibrium, association, and dissociation of 2'GMP and 3'GMP with Ribonuclease T1 at pH 5.3., **Biochimica et Biophysica Acta** 1073:357-365, 1991.
15. MacKerell, A.D., Jr., Principles and methods in molecular modeling and dynamics of biologically active peptides: Application to neuropeptide Y., **Methods in Enzymology** 202:449-470, 1991.
16. MacKerell, A.D., Jr. and Karplus, M., Importance of attractive van der Waals contribution in empirical energy function models for the heat of vaporization of polar liquids., **Journal of Physical Chemistry** 95:10559-10560, 1991.
17. Uvdal, P., MacKerell, A.D., Jr., and Wiegand, B.C., Intramolecular vibrational coupling of adsorbates probed using HREELS and *ab initio* calculations: ethoxides absorbed on Mo(110)., **Journal of Electron Spectroscopy and Related Phenomena**, 64/65: 193-199, 1993.
18. Yang, B., Wright, J., Eldefrawi, M.E., Poi, S.,and MacKerell, A.D., Jr., Conformational, aqueous solvation and pK_a contributions to the binding of cocaine, WIN and a WIN vinyl analog. **Journal of the American Chemical Society**, 116:8722-8732, 1994.
19. MacKerell, A.D., Jr., Molecular dynamics simulation analysis of a sodium dodecyl sulfate micelle in aqueous solution: Decreased fluiditiy of the micelle hydrophobic interior., **Journal of Physical Chemistry**, 99:1846-1855, 1995

20. MacKerell, A.D., Jr., Sommer, M.S. and Karplus, M., "pH Dependence of binding reactions from free energy simulations and macroscopic continuum electrostatic calculations: Application to 2'GMP/3'GMP binding to ribonuclease T1," **Journal of Molecular Biology**, 247:774-807, 1995.
21. Uvdal, P., MacKerell, A.D., Jr., Wiegand, B.C. and Friend, C.M., Surface-induced alteration of adsorbate intramolecular vibrational coupling: 2-propoxide on Mo(110) as determined by ab initio calculations and experiments., **Physical Review B**, 51:7844-7848, 1995.
22. MacKerell, Jr. A.D., Wiorkiewicz, J.K. and Karplus, M., All-atom empirical energy function for the simulation of nucleic acids., **Journal of the American Chemical Society**, 117:11946-11975, 1995.
23. Yin, D. and MacKerell, A.D., Jr., *Ab initio* calculations on the use of Helium and Neon as probes of van der Waals surfaces of molecules., **Journal of Physical Chemistry**, 100:2588-2596, 1996.
24. Ho, L.L., MacKerell, A.D., Jr. and Bash, P.A., Proton and Hydride Transfers in Solution (I): Hybrid, QM/MM Free Energy Perturbation Study. **Journal of Physical Chemistry**, 100:4466-4475, 1996.
25. Bash, P.A., Ho, L.L., MacKerell, A.D., Jr., Levine, D. and Hallstrom, P., Progress toward Chemical Accuracy in the Computer Simulations of Condensed Phase Reactions. **Proceedings of the National Academy of Sciences, USA**, 93: 3698-3703, 1996,
26. Feng, M.-H., Philippopoulos, M., MacKerell, A.D., Jr. and Lim, C., Structural Characterization of the Phosphotyrosine Binding Region of a High-Affinity SH2 Domain-Phosphopeptide Complex by Molecular Dynamics Simulation and Chemical Shift Calculations., **Journal of the American Chemical Society**, 118: 11265-11277, 1996.
27. Pavelites, J.J., Bash, P.A., Gao, J., and MacKerell, A.D., Jr., A Molecular Mechanics Force Field for NAD^+, NADH and the Pyrophosphate Groups of Nucleotides., **Journal of Computational Chemistry**, 18: 221-239, 1997.
28. Li, Y., MacKerell, A.D., Jr., Egorin, M.J., Ballesteros, M.F., Rosen, D.M., Wu, Y.-Y., Blamble, D.A. and Callery, P.S., Structure-Function Relationships of Polyamine Transport Inhibitors in L1210 Murine Leukemia Cells, **Cancer Investigation**, 57: 234-239, 1997.
29. MacKerell, A.D., Jr., Influence of Magnesium Ions on Duplex DNA Structural, Dynamic and Solvation Properties. **Journal of Physical Chemistry B**, 101: 646-650, 1997.
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33. Yin, D. and MacKerell, A.D., Jr., "Combined *Ab initio*/Empirical Approach for the Optimization of Lennard-Jones Parameters," **Journal of Computational Chemistry,** 19: 334-338, 1998.
34. Lieske, S., Yang, B., Eldefrawi, M.E. and MacKerell, A.D., Jr., and Wright, J., (-)3β-Substituted Ecgonine Methyl Esters as Inhibitors for Cocaine Binding and Dopamine Uptake., **Journal of Medicinal Chemistry**, 41: 864-876, 1998.

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48. Ásmundssson, R., Uvdal, P. and MacKerell, A.D., Jr., Binary combination and overtone modes in the C-H stretch region in ethoxy adsorbed on Cu(100): Experimental and calculated vibrational spectra., **Journal of Chemical Physics**, 113:1258-1267, 2000.

49. Wang, P., Nicklaus, M.C., Marquez, V.E., Brank, A.S., Christman, J., Banavali, N.K. and MacKerell, A.D., Jr., Use of Oligodeoxyribonucleotides with Conformationally Constrained Abasic Sugar Targets to Probe the Mechanism of Base Flipping by HhaI DNA (Cytosine C5)-Methyltransferase., **Journal of the American Chemical Society**, 122:12422-12434, 2000.
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51. Marquez, V.E., Wang, P., Nicklaus, M.C., Maier, M., Manoharan, M., Christman, J.K., Banavali, N.K., and MacKerell, A.D., Jr., Inhibtion of (Cytosine C5)-Methyltransferase by Oligonucleotides Containing Flexible (Cyclopentane) and Conformationally Constrained (Bicyclo[3.1.0]hexane) abasic sites., **Nucleosides, Nucleotides and Nucleic Acids**, 20:451-450, 2001.
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58. Chen, I-J., Neamati, N. and MacKerell, Jr. A.D., Structure-Based Inhibitor Design Targeting HIV-1 Integrase., **Current Drug Targets - Infectious Disorders**, 2: 217-234, 2002.
59. Foloppe, N., Hartmann, B., Nilsson, L. and MacKerell, A.D., Jr.,, Intrinsic Conformational Energetics Associated with the Glycosyl Torsion in DNA: a Quantum Mechanical Study, **Biophysical Journal**, 82: 1554-1569, 2002.
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64. Huang, N. Banavali, N.K., and MacKerell, A.D., Jr., Protein-facilitated base flipping in DNA by cytosine-5-methyltransferase. **Proceedings of the National Academy of Sciences, USA**, 100: 68-73, 2003, PMID: 12506195.
65. Chen, W., Wu, H,. Bernard, D., Metcalf, M.D., Deschamps, J., Flippen-Anderson, J., MacKerell, A.D., Jr., and Coop, A., Rearrangement of 5-Trimethylsilylthebaine on Treatment with L-Selectride: An Efficient Synthesis of (+)-Bractazonine, **Journal of Organic Chemistry**, 68: 1929-1932, 2003.
66. Bernard, D., Coop, A. and MacKerell, A.D., Jr. , 2D Conformationally Sampled Pharmacophore: A Novel Approach to Ligand Based Pharmacophore Development Applied to δ Opioid Agonists and Antagonists, **Journal of the American Chemical Society**. 125: 3103-3107, 2003.
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68. Lamoureux, G., MacKerell, A.D., Jr., Roux, B., A simple polarizable model of water based on classical Drude oscillators, **Journal of Chemical Physics**, 119: 5185-5197, 2003
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71. MacKerell, A.D., Jr., Feig, M. and Brooks, III, C.L., "Improved treatment of the protein backbone in empirical force fields," **Journal of the American Chemical Society**, 126:698-699, 2004.
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4) "Targeting NAD Biosynthesis in Bacterial Pathogens" MacKerell Jr., A.D., Zhang, H., and Osterman, A. US Patent Office Publication Number US 2012-0190708, WO 2011-006158.

5) “Defensin-Like Molecules as Novel Antimicrobial Agents,” De Leeuw, E and MacKerell Jr., A.D., PCT Patent Application Number: US patent application # 61/656,039, WO 2012-061767, UMB Docket Number: ED-2010-066.
6) “GTP Binding Regulators of Leucine-rich Repeat Kinase-2 (LRRK2) for Treatment of Parkinson’s Disease,” Smith, W., and MacKerell Jr., A.D., US Provisional Patent application # 61/555,660, UMB Docket #: WS-2012-018
7) “Site-Specific Fragment Identification Guided by Single-Step Free Energy Perturbation Calculations.” MacKerell Jr., A.D. and Raman, E.P. PCT Application filed March 20, 2013, UMB Docket Number AM-2012-069.
8) “Novel Mixed Mu Agonist, Delta Antagonist Opioid Analgesics with Reduced Tolerance Liabilities and Uses Thereof,” Coop, A., MacKerell, A.D., Jr. and Matsumoto, R., US Patent application # 61/774,128, UMB Docket: AC-2013-055

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1) “Method of Designing an Agent that Mimics a Functional Epitope,” Hayashi, J. and MacKerell, Jr., A.D, U.S. Patent Application 09/673,693 (inactive)
2) “Method for Treating Disease Due to Nonsense Mutation” Matsuga, R., Shiozuka, M., and MacKerell, A.D., Jr., U.S. Patent Application#: 12/307,027, PCT/JP2007063436 (inactive)
3) “Immunomodulatory Compounds that target and inhibit the pY+3 binding site of tyrosine kinase p56 LCK SH2 domain” MacKerell, A.D., Jr. Hayashi, J., Nagarsekar, A., Macias, A., and Huang, N., U.S. Patent Application 10/582,640, International Patent Application PCT/US2003/39501 (inactive)
4) “Inhibitors of Extracellular Signal-Regulated Kinase Docking Domains and Uses Thereof” Shapiro, P.S. and MacKerell, A.D., Jr., US Patent Application Number: 11/543,491, filed 10/5/06, International Patent Application PCT/US2006/011536, Publication # WO2006/105237 (inactive)
5) “Balancing Target Flexibility and Target Denaturation in Computational Fragment-Based Inhibitor Discovery,” “ Foster, T.J., MacKerell Jr., A.D. and Guvench, O., Provisional Patent Application 61/603,630 (inactive)
6) “Regulation of RUNX2 Transcription of Factor-DNA Interactions Using Vitamin D3 (Cholecalciferol) Prohormone Activity” Passaniti, A., MacKerell Jr., A.D., Underwood, K. and Adaku, UMB Docket Number: AP-2012-053, US Provisional Patent Application Number: 61/577,724.

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Invited Lectures

1. "Dynamics of ribonuclease T1 and horse liver alcohol dehydrogenase: Combining experimental and theoretical information," European Society for Photobiology Meeting, Padova, Italy, 1987
2. "Structural and dynamics differences in the free and 2'GMP enzyme forms of ribonuclease T1,"First International Meeting on the Structure and Chemistry of Ribonucleases, Moscow, USSR, 1988
3. "Motivation and Validation for the use of Empirical Force Fields for Computational Studies of Biological Systems," First World Congress on Medicine, Public Health and Biotechnology. Austin, Texas, 1994.

4. “Validation of the use of Empirical Force Fields for Computational Studies of Biological Systems” Department of Microbiology and Immunology, School of Medicine, University of Maryland at Baltimore, Baltimore, MD, 1994.
5. “Validation of the Use of Empirical Force Fields for Computational Studies of Biological Systems” 8th Middle Atlantic Regional Meeting of the Americal Chemical Society Univeristy of Maryland Baltimore County, Catonsville, MD, 1994.
6. “Empirical Force Field Development and Validation for Computational Studies of Biological Membranes,”208th American Chemical Society National Meeting, Washington D.C., 1994
7. “Molecular Dynamics Simulation Studies of Nucleic Acids,” Research Seminar, University of Maryland Cancer Center, Department of Developmental Therapeutics, School of Medicine, University of Maryland,Baltimore, Baltimore, MD, 1995
8. “Molecular Dynamics Simulation Studies of Nucleic Acids,” Molecular and Cell Biology Graduate Program Seminar Series, University of Maryland at Baltimore, Baltimore, MD, 1995
9. “Molecular Dynamics Simulation Studies of Nucleic Acids,” Department of Chemistry and Biochemistry Seminar Series University of Maryland Baltimore County, Catonsville, MD, 1995
10. “Methodological Developments in the Optimization of Lennard-Jones Parameters for Empirical Force Field Calculations,” Biophysic Laboratory, Center for Biologics Evaluation & Research, Food and Drug Administration and Laboratory of Structural Biology, Division of Computer Research & Technology, NIH, Bethesda, MD, 1995
11. “Empirical Force Field Parameterization and Simulations of Nucleic Acids,” Laboratory of Medicinal Chemistry, National Cancer Institute, NIH, Bethesda, MD, 1995
12. “Molecular Dynamics Simulation Studies of the EcoRI restriction site dodecamer,” Department of Chemistry, University of Houston, Houston, Texas, 1995
13. "An all-atom empirical energy function for the simulation of nucleic acids, " 210th American Chemical Society National Meeting, Chicago, Il,1995.
14. "MD simulations of the EcoRI recognition sequence in solution: Influence of counterions on stability," 210th American Chemical Society National Meeting, Chicago, Il.,1995.
15. "Combined ab initio/empirical approach for the optimization of Lennard-Jones parameters.” 210th American Chemical Society National Meeting, Chicago, Il,1995.
16. “Computational Approaches to the Study of Biological Systems” Department of Chemistry, Towson State University, Towson, MD, 1995
17. “Empirical Force Field Calculations of Nucleic Acids: Parametrization and Application” Center for Structural Biology Department of Bioscience at Novum, Karolinska Institutet, Huddinge, Sweden, 1996.
18. “Empirical Force Field Calculations of Nucleic Acids: Parametrization and Application” Section de Biphysique des Protéines et de Membranes, Commissariat a l’Energie Atomique, CEA-Saclay, Saclay, France, 1996.
19. “Empirical Force Field Calculations of Nucleic Acids: Parametrization and Application” Laboratoire de Chimie Biophysique, Institut le Bel, Universite Louis Pasteur, Strasbourg, France, 1996.
20. “Validation of Empirical Force Fields Based on Crystal Calculations” 212th American Chemical Society National Meeting, Orlando, FL, 1996.

21. “Use of Ab Initio Calculations to Aid in the Interpretation of the Influcence of Surface Adsorption on the Vibrational Spectra of Alkoxides” 212th American Chemical Society National Meeting, Orlando, FL. 1996.
22. “Lennard-Jones Parameters of Alkanes and Alkenes Based on a Combined Ab Initio-Empirical Optimization Procedure” 212th American Chemical Society National Meeting, Orlando, FL, 1996.
23. “Relationship of Small Molecule Based Parameter Optimization to Condensed Phase Calculations on Proteins and Nucleic Acids” Center Européen de Calcul Atomique et Moléculaire, Workshop: Potential functions for simulation of biomolecules, Lyon, France, 1996.
24. “MD based Potential of Mean Force Calculations on DNA under Tensile Force.” Chemistry Division, Naval Research Laboratory, Washington, DC. 1997
25. “MD based Potential of Mean Force Calculations on DNA under Tensile Force.” Center for Molecular Modeling, Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 1997
26. “Potential of Mean Force Calculations on DNA under Tensile Force.” Center for Advanced Research in Biotechnology, University of Maryland, Rockville, MD, 1997
27. “Structure, Force and Energy of a Double-Stranded DNA Oligonucleotides Under Tensile Loads,” Swiss Federal Institute of Technology, Lausanne, Switzerland, 1997.
28. “Structure, Force and Energy of a Double-Stranded DNA Oligonucleotides Under Tensile Loads” Center Européen de Calcul Atomique et Moléculaire, Workshop: Nucleic Acids, Lyon, France, 1997.
29. “Structure, Force and Energy of a Double-Stranded DNA Oligonucleotides Under Tensile Loads” Department of Physiology, School of Medicine, Johns Hopkins University, Baltimore, MD, 1997.
30. “Importance of microscopic contributions to condensed phase macroscopic properties in empirical force field calculations” Computational Chemistry Gordon Conference, Tilton, NH, 1998
31. “Developments in the CHARMM All-Atom Empirical Energy Function for Biological Molecules” 216th American Chemical Society National Meeting, Boston, MA, 1998
32. “Importance of microscopic contributions to condensed phase macroscopic properties in empirical force field calculations” Making and Breaking Potentials, UK Cooperative Computational Project #5 Annual Meeting, Edinburgh, Scotland, 1998
33. “Importance of microscopic contributions to condensed phase macroscopic properties in empirical force field calculations: Application to Nucleic Acids” Department of Chemistry, Georgetown Medical School, Georgetown University, Georgetown, VA, 1998
34. “Mechanical and Environmental Contributions to Opening of Duplex DNA in the TATA Box and Related Oligomers Investigated via Potential of Mean Force Calculations.” Molecular Modeling Interest Group, National Institutes of Health, Bethesda, MD, 1999.
35. “CHARMM empirical force field for biological molecules: Overview of optimization procedures with emphasis on lipid bilayers.” Center Européen de Calcul Atomique et Moléculaire, Workshop: Molecular Dynamics Simulations of Lipid Membranes and Membrane Associated Proteins, Lyon, France, 1999.
36. “Optimization of the CHARMM all-atom nucleic acid force field and investigation of the energetics of DNA deformation.” Department of Biochemistry, University of Zürich, Zürich, Switzerland, 1999.

37. “Optimization of the CHARMM all-atom nucleic acid force field.” Laboratoire de Chimie Biophysique, Institut le Bel, Universite Louis Pasteur, Strasbourg, France, 1999.
38. “HIV Integrase: Identification of Novel Inhibitors and Analysis of Enzyme-Inhibitor Interactions via Ligand Docking.” School of Pharmacy, West Virginia University, Morgantown, WV, 2000.
39. “Balancing Microscopic Contributions with Macroscopic Observables in Empirical Force Fields: Application to Nucleic Acids.” National Institute of Occupational Safety and Health, Morgantown, WV, 2000.
40. “Balancing Microscopic Contributions with Macroscopic Observables in Empirical Force Fields. Application to Nucleic Acids” Department of Chemistry, University of York, York, UK, 2000
41. “Advances in the CHARMM all-atom force field for biological molecules” Canadian Computational Chemistry Conference 4, Bishop University, Quebec, Canada, 2000.
42. “Advances in the CHARMM all-atom force field for biological molecules” 220th American Chemical Society National Meeting, Washington, DC, 2000.
43. “Use of Oligodeoxyribonucleotides with Conformationally Constrained Abasic Sugar Targets to Probe the Mechanism of Base Flipping by *HhaI* DNA (Cytosine C5)-Methyltransferase” Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, 2000
44. “Overview of the CHARMM all-atom force field for biological molecules” 4th Biannual Structural Biology Symposium, Institute of Molecular Biophysics, Florida State University, Tallahassee, FL, 2001
45. “Recent Advances in Biomolecular Molecular Dynamics Simulations: DNA Conformational Transitions and the Impact of Protein Binding” School of Chemical Engineering, Purdue University, West Lafayette, IN, 2001.
46. “Computational Studies of Base Flipping In DNA and Impact of Binding with the (Cytosine-5) Methyltransferase from *Hha*I” Department of Chemistry and Biochemisty, Duquesne University, Pittsburgh, PA, 2001
47. “Base Flipping in DNA and the Impact of Binding to (Cytosine-5) Methyltransferase from *Hha*I” Department of Chemistry, Kansas University, Lawrence, KS, 2001
48. “*Ab initio* Quantum Mechanical Analysis of Nucleic Acid Components” DIMACS Workshop on DNA Sequence and Topology, DIMACS Center, Rutgers University, Piscataway, NJ, 2001.
49.”Computational Studies of Base Flipping In DNA” Laboratory of Medicinal Chemistry, National Cancer Institute, National Institutes of Health, Frederick, MD, 2001.
50. “Energetic and Structural Details of Base Flipping from Duplex DNA” Horizons in Biophysics 2001, Royal Swedish Academy of Sciences, Nobel Institute of Chemistry, Stockholm, Sweden, 2001.
51. “Energetic and Structural Details of Base Flipping from Duplex DNA” Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, 2001.
52. “Drude Oscillator as a Model for Electronic Polarization in Empirical Force Fields: Application to Dimethylphosphate” Workshop on Polarizability for Biomolecular Simulation, Snowbird, Utah, 2001.
53. “CHARMM Force Fields: Approaches, Recent Developments and the Misery….” Department of Chemistry and Biochemistry, University of California, San Diego, CA, 2002.

54. " Recent developments in the CHARMM all-atom force field for nucleic acids" 223rd American Chemical Society National Meeting, Orlando, Fl., 2002
55. CHARMM Force Fields: Approaches, Recent Developments and the Misery…." Accelyrs Corporation, San Diego, CA, 2002.
56. "Base Flipping in DNA: Facilitation by the Enzyme Cytosine-5-Methyltransferase" Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA, 2002.
57. "Improved representation of protein backbone conformational energetics and condensed phase simulations of dimethylphosphate using the Shell Model to treat electronic polarizability," CHARMM Meeting, Department of Chemistry, Harvard University, Cambridge MA, 2002.
58. "Computational Studies of Base Flipping Alone and Complexed to the Cytosine-5-Methyltransferase from *Hha*I" Diffraction Methods In Structural Biology, Gordon Research Conference, New London, CT, 2002
59. "CHARMM biomolecular force field: Recent developments and future directions," American Chemical Society National Meeting, Boston, MA, 2002
60. "Empirical Force Fields: Overview, parameter optimization & applications," Department of Physics, University of Cyprus, Nicosia, Cyprus, 2003
61. "Force Fields" Short Course on Force Fields and Molecular Dynamics," Quantum Theory Project 43rd Sanibel Symposium, University of Florida, St. Augustine, Fl, 2003
62. "Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from *Hha*I," DNA and beyond: Structure, Dynamics and Interactions, École Polytechnique Fédérale de Lausanne, Laussane, Switzerland, 2003.
63. "Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from *Hha*I," Laboratory of Biophysical Chemistry Seminar Series, National Heart, Lung and Blood Institute, NIH, Bethesda, MD, 2003.
64. "Computer-Aided Drug Design: Ligand- and Target-Based Applications," Chemistry Group, National Institute of Drug Abuse, NIH, Baltimore, MD, 2003.
65. "CHARMM biomolecular force field: Recent developments and future directions," Annual CHARMM Developers Meeting, The Scripps Reseach Institute, LaJolla, CA, 2003.
66. "Improved Treatment of the Protein Backbone Conformation in the CHARMM All-atom Force Field," Computing for Biology, IBM-BNL Blue-Gene Science Workshop, Stony Brook, NY, 2003.
67. "CHARMM all-atom empirical force field for biomolecules: Recent enhancements and progress towards inclusion of electronic polarizability" Theoretical and Computational Biophysics Seminar, Beckman Institute, University of Illinois, Urbana-Champaign, IL, 2003
68. "Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from *Hha*I," Department of Chemistry Seminar Series, Pennsylvania State University, State College, PA, 2003
69. "Computational methods used in drug discovery" Department of Medical and Research Technology, University of Maryland School of Medicine, Continuing Education Credits, Baltimore, MD, 2003
70. "Base Flipping in DNA: Accessing Millisecond Events via MD-based Potential of Mean Force Calculations," 48th Annual Meeting of the Biophysical Society, Baltmore, MD, USA, February 2004

71. “Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from HhaI,” 2004 President's Meeting, International Society of Quantum Biology and Pharmacology, Como, Italy, June 2004.
72. “Parameters, parameters, parameters,” Annual CHARMM Developers Meeting, Harvard University, Cambridge, MA, July 2004
73. “Enhancements and Extensions of the CHARMM Biological Empirical Force Fields” Frontiers in Computational Biophysics and Drug Design, Army Research Laboratories Workshop, Beltsville, MD, October 2004
74. “Enhancements and Extensions of the CHARMM Biological Empirical Force Fields” Keck Computational and Theoretical Biology Symposium, Rice University, Houston, TX, December, 2004
75. “Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from *Hha*I” World Association of Theoretically Oriented Chemists, 2005 International Meeting, Cape Town, South Africa, January, 2005
76. “Computer-Aided Drug Design: Ligand- and Target-Based Approaches” Howard University, School of Pharmacy, Department of Pharmaceutical Sciences Seminar, March 2005
77. “Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from *Hha*I” Molecular Biophysics Seminar Series, Wesleyan University, Middletown, CT, April 2005.
78. “Progress in the CHARMM force fields; Extension to polarizable model based on the classical Drude oscillator,” Annual CHARMM meeting, Weill Medical College, Cornell University, New York, NY, July 2005
79. “Improvements in the CHARMM all-atom force fields for biomolecules” 230th National American Chemical Society Meeting, Washington, DC, August 2005
80. “MD simulation Studies of Base Flipping in DNA,” International Society of Quantum Biology and Pharmacology Gilda Lowe Memorial Meeting, Staten Island, New York, October 2005.
81. “Structure-function relationships of nucleic acids and protein-nucleic acid complexes studied via MD simulations” Bioinformatics Institute Visiting Scientist Lecture Series, Singapore, March 2006.
82. “Computer-aided drug design: Ligand-based approaches on δ-opioid ligands” Bioinformatics Institute Visiting Scientist Lecture Series, Singapore, March 2006.
83. “Computer-aided drug design: Target-based approaches with emphasis on protein-protein interactions” Bioinformatics Institute Visiting Scientist Lecture Series, Singapore, March 2006.
84. “Overview of the CHARMM all-atom force fields including the additive and classical Drude polarizable models,” Validating Modeling and Experimental Methods to Enable Drug Discovery, National Institute of Standards and Technology, Gaithersburg, MD., April, 2006.
85. “Overview of the CHARMM all-atom force fields including the additive and classical Drude polarizable models” Center for Bioinformatics, University of Kansas, Lawrence, Kansas, April, 2006.
86. “MD simulation studies of base flipping in DNA alone and in the presence of the (cytosine-C5)-methyltransferase from HhaI” Department of Chemistry, University of Kansas , Lawrence, Kansas, April, 2006.
87. “CHARMM force fields: 2006” Annual CHARMM Developers Meeting, Harvard University, Cambridge, MA, July 2006.

88. “MD simulation studies of base flipping in DNA alone and in the presence of the (cytosine-C5)-methyltransferase from HhaI” MMTSB Workshop, The Scripps Research Institute, LaJolla, California, August, 2006.
89. “Polarizable empirical force field based on the classical Drude oscillator model” Computational Chemistry Gordon Conference, Les Diablerets, Switzerland, October 2006.
90. “Computer-Aided Drug Design; Targeting the Tyrosine Kinase p56Lck SH2 Domain” Structure Biology Program, St. Jude Children’s Hospital, Memphis, Tennessee. October 2006.
91. “Ligand-based drug discovery using CHARMM; Conformationally sampled pharmacophore (CSP)” Accelyrs User Meeting and Conference 2006, Baltimore, Maryland, November 2006.
92. “Overview of CHARMM force fields and extension to drug-like molecules” Accelyrs User Meeting and Conference 2006, Baltimore, Maryland, November 2006.
93. “Polarizable empirical force field based on the classical Drude oscillator model” Florida State University Workshop 2007 on “Quantitative Computational Biophysics”, Florida State University, Tallahassee, Florida, February 2007.
94. “Computational studies of base flipping in DNA alone and bound to the cytosine-5-methyltransferase from HhaI” Department of Biochemistry and Molecular Biophysics, University of Chicago, Chicago, Illinois, USA, March 2007
95. “Optimization and validation of a polarizable force field based on the classical Drude oscillator” 233rd American Chemical Society National Meeting, Chicago, Illinois, USA, March 2007
96. “Ongoing developments in the CHARMM force fields for lipids” Semiannual Membrane Meeting, University of Utah, Park City, Utah, June 2007
97. “CHARMM force fields: 2007,” Annual CHARMM Developers Meeting, University of Maryland, School of Pharmacy, Baltimore, Maryland, USA, July 2007.
98. “Towards a Polarizable Force Field for Macromolecules: Optimization of a Force Field Based on the Classical Drude Oscillator,” Modeling Interactions in Biomolecules III, Prague, Czech Republic, September, 2007
99. “Computational studies of base flipping in DNA bound to the cytosine-5-methyltransferase from HhaI” FEBS Workshop on “DNA and RNA Modification Enzymes,” Centre Paul Langevin, Aussois, France, September 2007
100. “Advances in the CHARMM force fields for biological and pharmaceutical compounds” Accelrys Science Forum, Cambridge, MA, USA, October 2007.
101. “Development of a polarizable force field based on the classical Drude oscillator” 16th Conference on Current Trends in Computational Chemistry (CCTCC), Jackson State University, Jackson, MS, USA, November, 2007.
102. “Computational studies of base flipping in DNA alone and bound to the cytosine-5-methyltransferase from HhaI,” Institute for Structural Biology and Drug Discovery, Virginia Commonwealth University, Richmond, VA, USA, November, 2007.
103. “Development of a polarizable force field based on the classical Drude oscillator” American Physical Society March Meeting 2008, New Orleans, LA. March, 2008
104. “Computational studies of base flipping in DNA bound to the cytosine-5-methyltransferase from HhaI” Baltimore Area Repair Symposium (BARS), Baltimore, MD, March 2008
105. “Introduction and overview of CADD capabilities” Computer-Aided Drug Design Forum, School of Pharmacy, University of Maryland, Baltimore, MD, June 2008.

106. “The additive and Drude-based polarizable CHARMM force fields” Annual CHARMM Developers Meeting, Harvard University, Cambridge, MA, July 2008.
107. “Development of a Polarizable Empirical Force Field Based on the Classical Drude Oscillator” International Society of Theoretical Chemical Physics - VI, Vancouver, Canada, July 2008
108. “Inclusion of free energies of solvation during force field optimization” American Chemical Society 236th National Meeting, Philadelphia, PA, August 2008
109. “Optimization of a Polarizable Empirical Force Field Based on the Classical Drude Oscillator”American Chemical Society 236th National Meeting, Philadelphia, PA, August 2008
110. “Development of a Polarizable Force Field for Biological Molecules Based on the Classical Drude Oscillator.” Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, October 2008
111. “Optimization of a Polarizable Empirical Force Field Based on the Classical Drude Oscillator (and more....).” Department of Pharmaceutical Sciences, School of Pharmacy, University of California San Fransisco, San Fransisco, CA, February 2009.
112. “Optimization of a polarizable force field based on the classical Drude oscillator and application to biological macromolecules,” 237th American Chemical Society National Meeting, Salt Lake City, Utah, March 2009.
113. “Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from *Hha*I” Department of Biomedical and Pharmaceutical Sciences, College of Pharmacy, University of Rhode Island, Kingston, Rhode Island, April 2009.
114. “CHARMM force fields: 2009,” Annual CHARMM Developers Meeting, Karolinska Institutet, Stockholm Sweden, June 2009
115. “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation,” Biomolecular Simulations: Advanced Methods and Applications, Karolinska Institutet, Stockholm Sweden, June 2009
116. “CHARMM General Force Field (CGenFF) for pharmaceutical compounds; Development and use in drug design,” Accelyrs Users Group Meeting, Tokyo, Japan, July 2009
117. “Optimization of a polarizable force field based on the classical Drude oscillator and application to biological macromolecules,” Biomolecular Modeling and Simulations, Safed, Summer Workshop, Research workshop of the Israel Science Foundation, Safed, Israel, September, 2009
118. “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation,” Department of Chemistry, State University of New York, Stony Brook, October 2009
119 “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation,” Structural Biology and Chemistry Symposium, Dedicated to the memory of Dr. Nikos M. Oikonomakos, Institute of Organic and Pharmaceutical Chemistry, National Hellenic Research Foundation, Athens, Greece, October 2009
120. “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation,” Department of Chemistry and Biochemistry, Biophysics Program, Ohio State University, Columbus, Ohio, November 2009.
121. “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation,” Department of Chemistry and Biochemistry, University of Maryland, Baltimore County, Catonsville, Maryland, February, 2010

121. “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation,” 54th Annual Meeting of the Biophysical Society, San Fransisco, CA, February 2010.
122. “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation” Centre de recherché en modélisation moléculaire (CERMM) Seminar, Concordia University, Montreal, Canada, March 2010.
123. “Optimization of a polarizable force field based on the classical Drude oscillator and application to biological macromolecules,” Advances in the Implementation of Polarizable Force Fields for Molecular Simulations,” Center Européen de Calcul Atomique et Moléculaire, CECAM-HQ-EPFL, Lausanne, Switzerland, June 2010.
124. “Polarizable Empirical Force Field based on the Classical Drude Oscillator: Validation via Peptide Folding Simulations,” International Society for Quantum Biology and Pharmacology President’s Meeting, Cetraro, Italy, June 2010.
125. “Site Identification by Ligand Competitive Saturation (SILCS): Computational free energy-based approach for optimization of ligand-protein interactions,” Department of Physiology & Biophysics, School of Medicine, Case Western Reserve University, Cleveland, Ohio, November, 2010
126. “Site Identification by Ligand Competitive Saturation (SILCS): Computational free energy-based approach for optimization of ligand-protein interactions,” Bergen Centre for Computational Sciences, Faculty of Mathematics and Natural Sciences, University of Bergen, Bergen, Norway, November, 2010.
127. “Optimization of a polarizable force field based on the classical Drude oscillator and application to biological macromolecules,” Quantum Theory Project, University of Florida, Gainesville, Florida, December, 2010.
128. “An Overview of Force Fields & Molecular Mechanics Force Field Parameter Optimization,” Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Mahidol University, Bangkok, Thailand, January, 2011.
129. “Optimization of a polarizable force field based on the classical Drude oscillator,” Molecular Biophysics Unit, Indian Institute of Science, Bangalore, India, January, 2011.
130. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model.” 241st American Chemical Society National Meeting, Anaheim, CA, March 2011.
131. “CHARMM all-atom additive force field for carbohydrates: Parameter optimization overview and utilization for simulations of heterogeneous systems.” 241st American Chemical Society National Meeting, Anaheim, CA, March 2011.
132. “CHARMM additive and polarizable force fields for biomolecules and medicinal compounds,” Bioleap Inc., Ewing, NJ, April 2011.
133. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model,” Unité de Bioinformatique Structurale, Institut Pasteur, Paris, France, May 2011.
134. “Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for optimization of inhibitors of protein-protein interactions including BCL6, ERK and S100B,” Institut Pasteur, Paris, France, May 2011.
135. “CHARMM additive and polarizable force fields for biomolecules and medicinal compounds,” Accelrys Inc. User Group Meeting, Jersey City, NJ, May 2011.

136. “Trials and tribulations of a being a principle investigator in a postdoctoral-fellow “dominated” laboratory,” Office of Career Development, University of Maryland, School of Medicine, Baltimore, MD, May 2011.
137. “A tale with no end: Ongoing developments in the CHARMM additive and Drude force fields,” Annual CHARMM developers Meeting, University of Wisconsin, Madison, WI, July 2011.
138. “Role of the 2'OH on RNA conformational heterogeneity; Relevance to nucleic acid force field optimization,” Center Européen de Calcul Atomique et Moléculaire, Workshop: Dynamics of Protein-Nucleic Acid Interactions: Integrating Simulations with Experiments, CECAM-ETHZ, Zurich, Switzerland, September 2011.
139. “A tale with no end: Ongoing developments in the CHARMM additive and Drude force fields,” Department of Biochemistry, University of Zurich, September, 2011.
140. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model,” Lausanne Biomolecular Modeling Seminars, Swiss Institute of Bioinformatics, Ecole Polytechnique Federale Lausanne, Laussanne, Switzerland, October, 2011
141. “Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for optimization of inhibitors of protein-protein interactions including BCL6, ERK and S100B,” Biozentrum, Basel, Switzerland, October, 2011.
142. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model,” Department of Physical Chemistry, University of Basel, Basel, Switzerland, October, 2011.
143. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model,” Competence Center for Computational Chemistry (C4) of ETH Zurich, the University of Zurich and the IBM Research Laboratory, Zurich, Switzerland, October, 2011.
144. “Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for optimization of inhibitors of protein-protein interactions including BCL6, ERK and S100B,” University of Southern Florida, Department of Chemistry, Tampa, Florida, November, 2011
145. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model,” Department of Physics and Astronomy, University of Delaware, Newark, Delaware, February, 2012.
146. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model,” Instituto de Química, Universidade de São Paulo, São Paulo, Brazil, March 2012.
147. “Computer-Aided Drug Design: Ligand-Based Approaches.” In the workshop on “Advanced Topics in Computational Biology – Agrochemical and Drug Design”, Embrapa Agriculture Informatics, University of Campinas, UNICAMP, Campinas, São Paulo, Brazil, April, 2012.
148. “The CHARMM Force Field,” Center Européen de Calcul Atomique et Moléculaire, Workshop: Advances in Biomolecular Modelling and Simulations using CHARMM, University College Dublin, Dublin, Ireland, June 2012.
149. “Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for optimization of inhibitors of protein-protein interactions including BCL6, ERK and

S100B," University of Maryland Greenebaum Cancer Center, Molecular and Structural Biology Program, Baltimore, MD, June 2012.

150. "Contribution of the 2'-hydroxyl to the conformational properties of RNA," President's Meeting of the International Society of Quantum Biology and Pharmacology, Stockholm Sweden, June 2012
151. "Ongoing developments in the CHARMM additive and Drude force fields," Annual CHARMM developers Meeting, Computational Biophysics Section of the Laboratory of Computational Biology, National Heart, Blood and Lung Institute, National Institutes of Health, Rockville, MD, July 2012.
152. "Towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model," Computational Chemistry Gordon Conference, Mount Snow, Vermont, July 2012
153. "From Balls on Springs to Drugs and Things," University of Maryland Baltimore Research of the Year Seminar, Baltimore, MD, October, 2012
154. "Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for optimization of inhibitors of protein-protein interactions including BCL6, ERK and S100B," Sealy Center for Structural Biology and Molecular Biophysics, University of Texas Medical Branch, Galveston, TX, October, 2012
155. "Identification and Optimization of Inhibitors of Protein-Protein Interactions: ERK, S100B and BTB domain Containing Proteins" Department of Pharmacology, Weill Cornell Medical School, New York, NY, December, 2012
156. "Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model" Physics and Chemistry Seminar Series, Wake Forest University, Winston-Salem, NC, February, 2013
157. "Contribution of the 2'-hydroxyl to the conformational properties of RNA," University of Maryland, College Park, Department of Chemistry and Biochemistry Seminar, College Park, MD, February, 2013
158. "Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for optimization of inhibitors of protein-protein interactions including BCL6, ERK and S100B," Institute of Bioscience & Biotechnology Research, Rockville, MD, February, 2013
159. "Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model" Center for Molecular Biophysics, Oak Ridge National Laboratory, Oak Ridge, TN, March, 2013
160. "Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model" 245th American Chemical Society National Meeting, New Orleans, LA, April 2013.
161. "Site Identification by Ligand Competitive Saturation (SILCS): Mapping fragment binding sites including consideration of protein flexibility and fragment desolvation using an explicit solvent representation" 245th American Chemical Society National Meeting, New Orleans, LA, April 2013.
162. "Intrinsic contribution of the 2'-hydroxyl to RNA conformational heterogeneity," 245th American Chemical Society National Meeting, New Orleans, LA, April 2013.
163. "Site Identification by Ligand Competitive Saturation (SILCS): Structure-Based Free Energy Computational Approach for Ligand Discovery and Optimization," Cambridge Healthtech Institute's 8th Annual Drug Discovery Chemistry Meeting, San Diego, CA., April 2013.

164. “Site Identification by Ligand Competitive Saturation (SILCS): Structure-Based Free Energy Computational Approach for the Identification and Optimization of Ligands Targeting Proteins including Inhibitors of Protein-Protein Intearctions,” Drug Discovery & Therapy World Congress 2013, Boston, MA, USA, June 2013.
165. “Site Identification by Ligand Competitive Saturation (SILCS): Structure-Based Free Energy Computational Approach for Ligand Discovery and Optimization,” Cambridge Healthtech Institute and BIO-IT World’s 13th Structure-Based Drug Design Meeting, Boston, MA, June 2013.
166. “RNA Conformational Heterogeneity,” RNA Dynamics, Telluride Scientific Research Conference, Telluride, CO, USA, July 2013.
167. “Site Identification by Ligand Competitive Saturation (SILCS): Computational approach to to the identification and optimization of ligands targeting proteins, RNA and other macromolecules,” 2nd International Conference on Medicinal Chemistry & Computer-Aided Drug Designing, Las Vegas, NV, USA, October 2013.
168. “Toward opioid analgesics with decreased adverse side effects: From ligand-based to GPCR-based computer-aided drug design,” The 16th Annual Goodman Lecture, The Department of Physiology and Pharmacology, Oregon Health & Sciences University, Portland, OR, USA, October 2013.